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Response of Dipicolinic Acid ($C_5H_5N(COOH)_2$) to Ultrafast Laser Pulses[1] PETRA SAUER, ROLAND ALLEN, Texas A&M University — Dipicolinic acid (DPA) and its salts are common constituents of bacterial spores, including those of anthrax. It has been proposed that such spores can be detected via spectroscopic techniques which employ ultrashort laser pulses. The development of these techniques should be enhanced by a detailed understanding of the microscopic processes that transpire when a molecule is subjected to femtosecond-scale pulses of various intensities, durations, and polarizations. We have recently developed a model that can be used to perform realistic simulations of the electronic and nuclear dynamics of biological molecules (containing carbon, hydrogen, oxygen and nitrogen) when they are subjected to such pulses. The bond lengths and vibrational frequencies for a variety of test molecules are in reasonable agreement with those obtained in experiment and *ab initio* calculations. Here we report results of simulations for DPA responding to femtosecond-scale laser pulses, with an analysis of the vibrational modes and electronic states which are most relevant for various choices of the laser pulse parameters.

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